Thermal transport properties of disordered spin-1/2 systems

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Abstract

This work studies heat transport of bond-disordered spin-1/2 chains. As an example, the XX case is analyzed, which corresponds to a model of noninteracting spinless fermions. Within the fermion representation, the single-particle eigenenergies are determined numerically, which allow one to compute transport coefficients. Since the ballistic transport properties of a clean chain are destroyed by disorder, the focus is on the frequency dependence of the thermal conductivity and on a qualitative comparison with the spin conductivity, both at finite temperatures.

Key words: Quantum spin systems, Transport properties, Disorder
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Motivated by recent experiments on transport properties of transition metal oxides [1], intense theoretical work has recently been devoted to the study of heat conduction in one-dimensional spin-1/2 systems such as the Heisenberg chain, frustrated chains, and spin ladders [2]. Among these systems, the anisotropic spin-1/2 chain exhibits ballistic thermal transport properties at all temperatures T due to its integrability [3]. The thermal conductivity diverges in the homogeneous case, signaled by a finite thermal Drude weight [4]. Here, the usual decomposition of the real part of the thermal conductivity κ into the Drude weight D_{th} and the regular part is utilized: $\mathrm{Re}\,\kappa(\omega) = D_{\mathrm{th}}\delta(\omega) + \kappa_{\mathrm{reg}}(\omega)$, ω being the frequency. Ballistic transport is expected to be destroyed by randomness in the exchange couplings, resulting in a vanishing Drude weight. Therefore, one is interested in the regular part $\kappa_{\mathrm{reg}}(\omega)$, from which the dc-conductivity can be extracted by extrapolating to $\omega = 0$.

In this contribution, the effect of bond disorder on the thermal conductivity of XX chains is studied numerically. This limiting case of the anisotropic spin-1/2 chain corresponds to free spinless fermions by means of a Jordan-Wigner transformation [5]. While particle transport in disordered fermion systems is a long-studied problem, closely related to the subject of localization (see, e.g., Ref. [6]), the thermal conductivity κ in these models has attracted less attention. Using bosonization, predictions were made for the concentration dependence of the thermal conductivity of spin-1/2 chains [7], and it could be very interesting to compare this to numerical results. Here, results for the frequency dependence of κ are presented for the case of *off-diagonal* disorder at finite temperatures.

The Hamiltonian in terms of spin-1/2 operators $S_l^{\pm,z}$ acting on site l and with periodic boundary conditions (PBC) reads:

$$H = \frac{1}{2}\sum_{l=1}^{N} J_l\,(S_l^+ S_{l+1}^- + h.c.)\,, \tag{1}$$

where N is the number of sites. It can equivalently be written in terms of fermionic operators $c_l^\dagger$:

$$H = \frac{1}{2}\sum_{l=1}^{N} J_l\,(c_l^\dagger c_{l+1} + h.c.)\,. \tag{2}$$

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In principle, a subtlety arises since the PBCs for the spin operators give rise to a nontrivial boundary term for the fermions, which depends on the number $\mathcal{N}$ of fermions [8]. This dependence, however, is neglected here, and PBC are imposed for all $\mathcal{N}$, since boundary effects can be expected to vanish for large system sizes.

Introducing a spinor $\psi^\dagger = (c_1^\dagger, \ldots, c_N^\dagger)$, the Hamiltonian can be written as $H = \psi^\dagger \mathcal{A} \psi$, where $\mathcal{A}$ is a symmetric $N \times N$ band matrix, with nonzero elements $A_{l,l+1} = J_l/2$ and $A_{1,N} = J_1/2$. Randomness in the J_l is therefore called off-diagonal disorder, while a spatially varying magnetic field realizes *diagonal* disorder.

While a transformation to momentum space diagonalizes H for the translationally invariant case ($J_l = J$), the computation of single-particle eigenenergies is still straightforward for random couplings (see, e.g., [8]). By means of a unitary transformation $\mathcal{U}$ with $c_l = \sum_\mu \mathcal{U}_{l\mu}\eta_\mu$ that diagonalizes the matrix $\mathcal{A}$, the Hamiltonian can be written as $H = \sum_\mu \epsilon_\mu \eta_\mu^\dagger \eta_\mu$, where ϵ_μ are the single-particle eigenenergies.

The energy current operator corresponding to Eq. (2) is $\mathcal{J} = (i/4)\sum_l (c_l^\dagger c_{l+2} - h.c.) = i\sum_{\mu\nu} \eta_\nu^\dagger \mathcal{J}_{\nu\mu}\eta_\mu$. Within linear response theory, $\kappa_{\rm reg}(\omega)$ is given by [6]:

$$\kappa_{\rm reg}(\omega) = \frac{\beta}{\omega} \sum_{\epsilon_\mu \neq \epsilon_\nu} |\mathcal{J}_{\nu\mu}|^2 \, [f(\epsilon_\mu) - f(\epsilon_\nu)] \, \delta(\omega - \Delta\epsilon) \,, \quad (3)$$

where $f(\epsilon) = 1/(\exp(\beta\epsilon) + 1)$ denotes the Fermi-function, $\beta = 1/T$, and $\Delta\epsilon = \epsilon_\nu - \epsilon_\mu$.

As an example, a Gaussian distribution of random couplings is considered: $P(J_l) \propto e^{-(J_l - J)^2/w^2}$, with $J = 1$ and $w = 0.2$. The choice of the distribution does not affect the results, quantitatively consistent results for $\kappa(\omega)$ are obtained with other P_l (e.g. box or binary distribution) by fixing the first moments of the distribution function. Figure 1 shows results for $\kappa_{\rm reg}(\omega)$ [panel(b)] and, for comparison, $\sigma_{\rm reg}(\omega)$ [panel(a)], which is the spin conductivity corresponding to the current operator $\mathcal{J}_{\rm s} = (i/2)\sum_l (c_l^\dagger c_{l+1} - h.c.)$. The parameters are $T/J = 0.5$ and $N = 1000, 5000$. An imaginary broadening of 10^{-4} was used. The overall form of both quantities is quite similar and resembles that known for $\sigma_{\rm reg}(\omega)$ [9]. Moreover, both curves exhibit a maximum at roughly the same frequency ($\omega/J \approx 0.015$ for the parameters of Fig. 1). Both finite-size effects and statistical fluctuations are small in the low-frequency limit.

The behavior of $\kappa_{\rm reg}(\omega)$ at low frequencies is of particular interest as it determines the dc-conductivity (see Refs. [10] for the case of clean spin systems). While the Drude weights vanish in the presence of disorder, the results of this work indicate finite dc-conductivities for both spin and thermal transport at finite temperatures. This is illustrated in the inset of Fig. 1. A more detailed analysis of the finite-size scaling as well as the temperature dependence will be presented elsewhere.

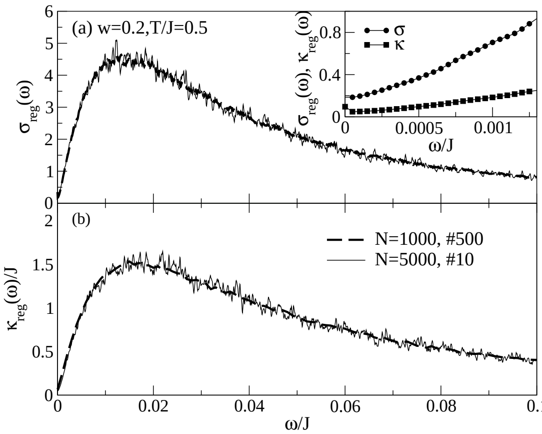

Fig. 1. Spin [panel (a)] and thermal conductivity [panel (b)] of an XX chain with a Gaussian distribution of random couplings J_l, centered around $J = 1$ and with a width of $w = 0.2$ (see text). Curves for $N = 1000(5000)$ sites and 500(10) random realizations for the same parameters are displayed. An imaginary broadening of 10^{-4} is used. The inset shows a blow-up of the low frequency region for the larger system size.

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References

[1] See, e.g.: A. V. Sologubenko et al., Phys. Rev. Lett. **84** (2000) 2714; C. Hess et al., Phys. Rev. B **64** (2001) 184305; K. Kudo et al., J. Phys. Soc. Jpn. **70** (2001) 437.

[2] See: X. Zotos and P. Prelovšek: in *Strong Interactions in Low Dimensions*, Kluwer Academic Publishers, 2004; and further references therein.

[3] X. Zotos, F. Naef, and P. Prelovšek, Phys. Rev. B **55** (1997) 11029.

[4] A. Klümper and K. Sakai, J. Phys. A **35** (2002) 2173; K. Sakai and A. Klümper J. Phys. A **36** (2003) 11617; F. Heidrich-Meisner et al., Phys. Rev. B **66** (2002) 140406; *ibid.* **68** (2003) 134436; *ibid.* **71** (2005) 184415.

[5] G. D. Mahan, Many-Particle Physics, Plenum Press, New York London, 1990.

[6] B. Kramer and A. MacKinnon, Rep. Prog. Phys. **56** (1993) 1469.

[7] C. I. Kane and M. P. A. Fisher, Phys. Rev. Lett. **76** (1996) 3192; A. V. Rozhkov and A. L. Chernyshev, Phys. Rev. Lett. **94** (2005) 087201.

[8] N. Laflorencie and H. Rieger, Eur. Phys. J. B **40** (2004) 201.

[9] O. Motrunich, K. Damle, and D. A. Huse, Phys. Rev. B **63** (2001) 134424.

[10] X. Zotos, Phys. Rev. Lett. **92** (2004) 067202; F. Heidrich-Meisner et al., Physica B **359-361** (2005) 1394.